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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 09	JAPIO to be reloaded August 25, 2002
NEWS 20	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 21	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 22	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded

NEWS EXPRESS	February 1 CURRENT WINDOWS VERSION IS V6.0d, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
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NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

Examiner Anderson 703-605-1157

FILE 'HOME' ENTERED AT 13:02:52 ON 21 AUG 2002

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 13:03:00 ON 21 AUG 2002

STRUCTURE FILE UPDATES: 20 AUG 2002 HIGHEST RN 444542-98-7
DICTIONARY FILE UPDATES: 20 AUG 2002 HIGHEST RN 444542-98-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

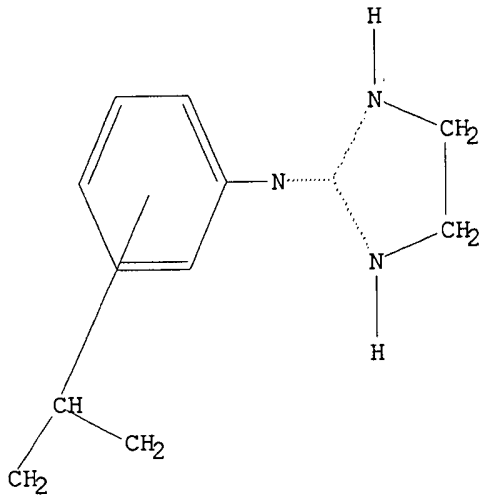
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10058456.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 H,X,O,C

G2 C,H,X

Examiner Anderson 703-605-1157

Structure attributes must be viewed using STN Express query preparation.

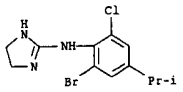
```
=> s l1 full
FULL SEARCH INITIATED 13:03:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  20061 TO ITERATE

100.0% PROCESSED   20061 ITERATIONS                          10 ANSWERS
SEARCH TIME: 00.00.03

L2            10 SEA SSS FUL L1

=> d scan
```

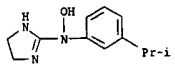
L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazol-2-amine, N-[2-bromo-6-chloro-4-(1-methylethyl)phenyl]-4,5-dihydro-, monohydrobromide (9CI)
MF C12 H15 Br Cl N3 . Br H



● HBr

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

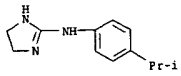
L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazol-2-amine, 4,5-dihydro-N-hydroxy-N-[3-(1-methylethyl)phenyl]-, monohydrochloride (9CI)
MF C12 H17 N3 O . Cl H



● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

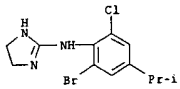
L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2-Imidazoline, 2-cumidino- (7CI, 8CI)
MF C12 H17 N3
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazol-2-amine, N-[2-bromo-6-chloro-4-(1-methylethyl)phenyl]-4,5-dihydro- (9CI)
MF C12 H15 Br Cl N3
CI COM

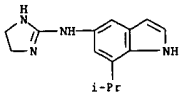


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Butanedioic acid, compd. with N-(4,5-dihydro-1H-imidazol-2-yl)-7-(1-methylethyl)-1H-indol-5-amine (1:1) (9CI)
MF C14 H18 N4 . C4 H6 O4

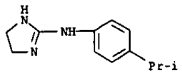
CM 1



CM 2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

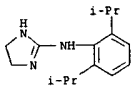
L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2-Imidazoline, 2-cumidino-, monohydrochloride (8CI)
MF C12 H17 N3 . Cl H



● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

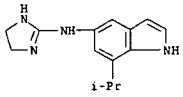
L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI)
MF C15 H23 N3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

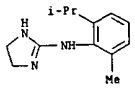
L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Indol-5-amine, N-(4,5-dihydro-1H-imidazol-2-yl)-7-(1-methylethyl)-(9CI)
MF C14 H18 N4
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

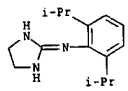
L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazol-2-amine, 4,5-dihydro-N-[2-methyl-6-(1-methylethyl)phenyl]-(9CI)
MF C13 H19 N3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 10 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzenamine, N-2-imidazolidinylidene-2,6-bis(1-methylethyl)-, monohydrochloride (9CI)
MF C15 H23 N3 . Cl H



● HCl

ALL ANSWERS HAVE BEEN SCANNED

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	140.66	140.87

FILE 'CAPLUS' ENTERED AT 13:04:22 ON 21 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 21 Aug 2002 VOL 137 ISS 8
FILE LAST UPDATED: 20 Aug 2002 (20020820/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s 12
L3 12 L2

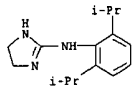
=> d ibib abs hitstr 1-12

L3 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:883550 CAPLUS
DOCUMENT NUMBER: 136:320707
TITLE: Three-Dimensional common-Feature hypotheses for octopamine agonist 2-(arylimino)imidazolidines
AUTHOR(S): Hirashima, Akinori; Morimoto, Masako; Kuwano, Eiichi; Taniguchi, Eiji; Eto, Morifusa
CORPORATE SOURCE: Department of Applied Genetics and Pest Management, Kyushu University, Faculty of Agriculture, Graduate School, Fukuoka, Higashi-ku, 812-8581, Japan
SOURCE: Bioorganic & Medicinal Chemistry (2001), Volume Date 2002, 10(1), 117-123
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three-dimensional pharmacophore hypotheses were built from a set of 10 octopamine (OA) agonist 2-(Arylimino)imidazolidines (AIIs), 2-(Arylimino)thiazolidines (AITs) and 2-(Arylimino)oxazolidines (AIOs). OA agonist activities were detd. using the adenylate cyclase assay in American cockroaches (P. americana). Among the 10 common-featured models generated by program Catalyst/HipHop, a hypothesis including a ring arom. (RA), a pos. ionizable (PI) and three hydrophobic aliph. (HpAl) features was considered to be important in evaluating the OA-agonist activity. Active OA agonist 2,6-Et2 AII mapped well onto all the RA, PI and HpAl features of the hypothesis. On the other hand, less active compds. were shown to be difficult to achieve the energetically favorable conformation which is found in the active mols. in order to fit the 3-D common-feature pharmacophore models. Taken together, 2,6-Et2-Ph and foramidine structures are important as OA agonists. The present studies on OA agonists demonstrate that a RA, a PI and three HpAl sites located on the mol. seem to be essential for OA-agonist activity.

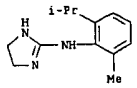
IT **63346-74-7 359668-33-0**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(QSAR for octopamine agonist (arylimino)imidazolidines)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 359668-33-0 CAPLUS
CN 1H-Imidazol-2-amine, 4,5-dihydro-N-[2-methyl-6-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2002 ACS (Continued)



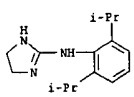
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:596828 CAPLUS
DOCUMENT NUMBER: 135:222824
TITLE: Identification of novel inhibitors of calling and in vitro [14C]acetate incorporation by pheromone glands of Plodia interpunctella
AUTHOR(S): Hirashima, Akinori; Eiraku, Tomohiko; Watanabe, Yasuyuki; Kuwano, Eiichi; Taniguchi, Eiji; Eto, Morifusa
CORPORATE SOURCE: Department of Applied Genetics and Pest Management, Faculty of Agriculture, Graduate School, Kyushu University, Fukuoka, 812-8581, Japan
SOURCE: Pest Management Science (2001), 57(8), 713-720
CODEN: PMSCFC; ISSN: 1526-498X
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Some octopamine agonists were found to suppress in vitro biosynthesis of the calling pheromone of the Indian meal moth, Plodia interpunctella. Isolated pheromone-gland prepns. incorporated sodium [14C]acetate at a linear rate for 3h when incubated with the pheromone biosynthesis activating neuropeptide (PBAN). This incorporation was dependent on the dose of PBAN (up to 0.5 .mu.M). Thin-layer chromatog. of a pheromone-gland ext. revealed quant. incorporation of radioactivity into a product exhibiting the same mobility as (Z,E)-9,12-tetradecadienyl acetate, the main component of the calling pheromone of P. interpunctella. Twenty-seven octopamine agonists were initially screened using a calling behavior bioassay of female P interpunctella. Four derivs. with activity in the nanomolar range were identified which were, in order of decreasing pheromonostatic activity: 2-(2,6-diethylphenylimino)thiazolidine > 2-(2,6-diethylphenylimino)oxazolidine > 2-(2,6-dimethylphenylimino)thiazolidine > 2-(2-ethylphenylimino)oxazolidine. These compds. also showed in vitro inhibitory activity in intracellular de novo pheromone biosynthesis. The results of the present study indicate that these derivs. could provide useful information in the characterization and differentiation of octopaminergic receptor types and subtypes.

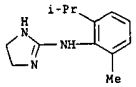
IT **63346-74-7P 359668-33-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and pheromonostatic activity of)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 359668-33-0 CAPLUS
CN 1H-Imidazol-2-amine, 4,5-dihydro-N-[2-methyl-6-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2002 ACS (Continued)



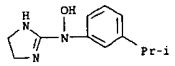
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:37784 CAPLUS
DOCUMENT NUMBER: 134:231513
TITLE: Synthesis, structure, and binding of some 2-imidazolines to rat brain alfa-1 and alfa-2-adrenergic receptors
AUTHOR(S): Saczewski, F.; Kobierska, E.; Debowski, T.; Charakchiewa-Minol, S.; Mokrosz, M.; Gdaniec, M.; Nowak, E.
CORPORATE SOURCE: Department of Chemical Technology of Drug and Organic Chemistry, Medical University of Gdansk, Pol.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2000), 333(12), 425-430
CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:231513

AB A series of novel 2-[(2-aminophenyl)imino]imidazolinium salts and N-benzyl-N-(4,5-dihydro-imidazol-2-yl)-O-methylhydroxylamine hydrochloride were prepd. and their structure was detd. by IR and NMR spectroscopic data as well as X-ray anal. of the imidazolinium azide salt of one of the compds. Binding evaluation for both .alpha.1- and .alpha.2-adrenergic receptors in rat brain prepns. of these compds. and previously described .alpha.-hydroxy-2-aryliminoimidazolines 11a-d, N-(4,5-dihydroimidazol-2-yl)-1,3-2-oxodihydrobenzimidazoles, 2-amino-N-(4,5-dihydroimidazol-2-yl)-benzimidazoles, and N-(4,5-dihydroimidazol-2-yl)-indoles was performed. Among the compds. tested, 2-[(2-amino-4,5-dichlorophenyl)imino]imidazolinium chloride showed highest binding affinity to .alpha.2-adrenoreceptors (Ki = 30 nM).

IT **330685-57-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(synthesis, structure, and binding of imidazolines to brain .alpha.1- and .alpha.2-adrenergic receptors)

RN 330685-57-9 CAPLUS
CN 1H-Imidazol-2-amine, 4,5-dihydro-N-hydroxy-N-[3-(1-methylethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

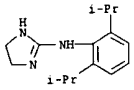
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:142505 CAPLUS
DOCUMENT NUMBER: 132:330832
TITLE: Three-dimensional molecular field analyses of octopaminergic agonists and antagonists for the locust neuronal octopamine receptor class 3
AUTHOR(S): Hirashima, A.; Nagata, T.; Pan, C.; Kuwano, E.; Taniguchi, E.; Eto, M.
CORPORATE SOURCE: Graduate School, Division of Bioresource and Bioenvironmental Sciences, Kyushu University, Fukuoka, Japan
SOURCE: Journal of Molecular Graphics & Modelling (2000), Volume Date 1999, 17(3/4), 198-206
CODEN: JMGMFI; ISSN: 1093-3263
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The quant. structure-activity relationship (QSAR) of a set of 70 octopaminergic agonists and 20 antagonists against octopamine receptor class 3 (OAR3) in locust nervous tissue was analyzed by mol. field anal. (MFA). MFA of these compds. evaluated effectively the energy between a probe and a mol. model at a series of points defined by a rectangular grid. Contour surfaces for the mol. fields are presented. These results provide useful information in the characterization and differentiation of octopaminergic receptor types and subtypes.

IT **63346-74-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(three-dimensional mol. field analyses of octopaminergic agonists and antagonists for locust neuronal octopamine receptor class 3)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



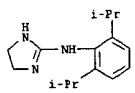
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:138409 CAPLUS
DOCUMENT NUMBER: 132:260196
TITLE: Prediction of distribution coefficients from structure. Comparison of calculated and experimental data for various drugs
AUTHOR(S): Tsantili-Kakoulidou, A.; Panderi, I.; Piperaki, S.; Csizmadia, F.; Darvas, F.
CORPORATE SOURCE: Department of Pharmacy, University of Athens, Athens, 157 71, Greece
SOURCE: European Journal of Drug Metabolism and Pharmacokinetics (1999), 24(3), 205-212
CODEN: EJDPD2; ISSN: 0378-7966
PUBLISHER: Medecine et Hygiene
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The efficiency of the program PrologD to predict distribution coeffs. (D) at any pH and pairing ion concn. has been tested using exptl. logD values for various drugs measured under std. conditions of buffers and ionic strength. Clonidine derivs., fluoroquinolones and .beta.-blockers were included as particular pharmacol. classes within the testing data set. Calcns. were performed using the three logP estn. options implemented in the program. PrologD proved to be very efficient and can be of great advantage in drug research. Prediction patterns and correlations between exptl. and calcd. data indicate acceptable results for more than 80% of the data. In addn., comparable studies using the different options permitted suggestions for the more suitable logP estn. method in respect of the particular classes of compds.

IT **63346-74-7**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(comparison of calcd. and exptl. data for various drugs in prediction of distribution coeffs. from structure)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:669819 CAPLUS
DOCUMENT NUMBER: 127:274156
TITLE: Neurotransmitter-receptors as targets for new insecticides
AUTHOR(S): Roeder, T.; Degen, J.; Dyczkowski, C.; Gewecke, M.
CORPORATE SOURCE: Zoologisches Insitut, Universitat Hamburg, Neurophysiologie, Hamburg, D-20146, Germany
SOURCE: New Strategies in Locust Control (1997), 219-223.
Editor(s): Krall, S.; Peveling, R.; Ba Diallo, D.
Birkhaeuser: Basel, Switz.
CODEN: 65EDA4
DOCUMENT TYPE: Conference
LANGUAGE: English

AB The locust neuronal octopamine receptor is believed to be an ideal target for highly specific insecticides. The authors characterized a no. of high affinity agonists of this receptor subtype. Using structure-activity relationships, the authors were able to optimize the structure of these compds. in terms of their affinities. A variety of these compds. show a high degree of specificity for insect octopamine receptors vs. vertebrate adrenergic receptors. The high affinity together with the high degree of specificity makes compds. such as the phenyliminoimidazolidines ideal starting points for the development of new insecticides.

IT **63346-74-7**, NC 20
RL: BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
(affinity for locust neuronal octopamine receptor)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

L3 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:594632 CAPLUS
DOCUMENT NUMBER: 127:262678
TITLE: Preparation of novel indoles and benzothiazoles for cloned human alpha 2 receptors
INVENTOR(S): Jeon, Yoon T.; Gluchowski, Charles
PATENT ASSIGNEE(S): Synaptic Pharmaceutical Corp., USA
SOURCE: PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9731636	A1	19970904	WO 1997-US3173	19970228
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5677321	A	19971014	US 1996-608598	19960229
CA 2246813	AA	19970904	CA 1997-2246813	19970228
AU 9720604	A1	19970916	AU 1997-20604	19970228
AU 704439	B2	19990422		
EP 900080	A1	19990310	EP 1997-908782	19970228
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2000506144	T2	20000523	JP 1997-531156	19970228
US 5948804	A	19990907	US 1997-926316	19970905
US 6040451	A	20000321	US 1999-345470	19990630
US 6159998	A	20001212	US 2000-492505	20000127
US 6303643	B1	20011016	US 2000-690620	20001017
US 2002049239	A1	20020425	US 2001-965944	20010928

PRIORITY APPLN. INFO.:
US 1996-608598 A 19960229
WO 1997-US3173 W 19970228
US 1997-926316 A1 19970905
US 1999-345470 A1 19990630
US 2000-492505 A1 20000127
US 2000-690620 A1 20001017

OTHER SOURCE(S): MARPAT 127:262678
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I-IV; R1-R3 = H, C1-7 alkyl, C2-7 alkenyl, alkynyl; R4-R6 = H, halo, Oh, etc.; R7 = H, NH, C1-7 alkyl, etc.; R8 = H, C1-7 alkyl, C2-7 alkenyl, etc.; R9 = H, Ph, C1-7 alkyl, etc.; X = CH2, O, NH, S] which are selective for cloned human alpha 2 receptors and therefore

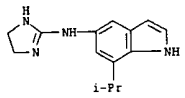
L3 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2002 ACS (Continued)

$HO_2C-CH_2-CH_2-CO_2H$

L3 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2002 ACS (Continued)
useful for lowering intraocular pressure, for treating presbyopia, migraine, hypertension, alc. withdrawal, drug addiction, rheumatoid arthritis, ischemic pain, spasticity, diarrhea, nasal congestion, urinary incontinence as well as for use as analgesics, sedatives, anesthetics, cognition enhancers and ocular vasoconstriction agents, were prepd. Thus, reaction of 7-bromo-5-aminoindole with 2-imidazoline-2-sulfonic acid (ISA) afforded 46% I [R1-R5 = H; R6 = Br; R7-R9 = H; X = N] which showed pEC50 of 9.36 at alpha 2 receptor.

IT **196204-74-7P 196204-75-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of novel indoles and benzothiazoles for cloned human alpha 2 receptors)

RN 196204-74-7 CAPLUS
CN 1H-Indol-5-amine, N-(4,5-dihydro-1H-imidazol-2-yl)-7-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 196204-75-8 CAPLUS
CN Butanedioic acid, compd. with N-(4,5-dihydro-1H-imidazol-2-yl)-7-(1-methylethyl)-1H-indol-5-amine (1:1) (9CI) (CA INDEX NAME)

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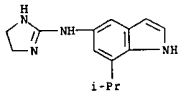
CRN 196204-74-7
CMF C14 H18 N4



CM 2

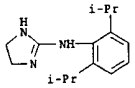
CRN 110-15-6
CMF C4 H6 O4

L3 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:303934 CAPLUS
DOCUMENT NUMBER: 122:77274
TITLE: Pharmacology of the octopamine receptor from locust central nervous tissue (OAR3)
AUTHOR(S): Roeder, Thomas
CORPORATE SOURCE: Zool. Inst., Univ. Hamburg, Hamburg, D-20146, Germany
SOURCE: British Journal of Pharmacology (1995), 114(1), 210-16
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Stockton
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The present study characterized highly effective agonists from different classes of compds. for the neuronal octopamine receptor (OAR3) of the migratory locust (Locusta migratoria L.). Biogenic amines and phenyliminoimidazolidines (PIIs) were employed for the study of structure-activity relationships. The highest affinity PIIs were predominantly those with the substitutions at the positions 2 and 4 of the phenolic ring (e.g. NC 7, KI = 0.3 nM, NC8, KI = 0.81 nM). Substitutions at these positions always had pos. effectives on the affinity of the resp. agonists. Substitutions at the positions 3, 5 and 6, however, always had neg. effects on the affinity. At the position one of the phenolic ring, heterocyclic substituents are preferred. Some PIIs had a more than 30 times higher affinity for OARs than for .alpha.-adrenoceptors which are the vertebrate homologues of the insect octopamine receptors. The only non-PII with subnanomolar affinity was the aminooxazlline deriv. AC 6 (KI = 0.92 nM). A variety of substances with known insecticidal activity such as chlordimeform, demethylchlordimeform, amitraz or AC 6 had high affinity for the locust neuronal octopamine receptor.

IT **63346-74-7**, NC 20
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(structure-activity relationship of agonists for locust neuronal octopamine receptor)

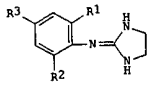
RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



L3 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:95240 CAPLUS
DOCUMENT NUMBER: 110:95240
TITLE: Preparation of 2-(phenylimino)imidazolidines as .alpha.1-adrenergic agonists
INVENTOR(S): Esser, Franz; Staehle, Helmut; Koeppe, Herbert; Speck, Georg; Mierau, Joachim; Pichler, Ludwig; Lehr, Erich
PATENT ASSIGNEE(S): Boehringer Ingelheim K.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 7 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3712385	A1	19881027	DE 1987-3712385	19870411

OTHER SOURCE(S): CASREACT 110:95240; MARPAT 110:95240
GI



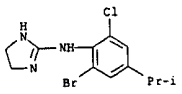
I

AB The title compds. [I; R1, R2 = F, Cl, Br, iodo; R3 = (substituted) C1-4 alkyl] and pharmaceutically acceptable salts were prepd. as CNS agents and cyto- and cardioprotectants. KSCN in acetone was treated with PhCOCl at 15.degree. and 2-chloro-4-isopropylaniline was added. The mixt. was refluxed 3.25 h to give 70.5% (2-chloro-4-isopropylphenyl)thiourea. The latter was sequentially refluxed with MeI in MeOH, refluxed with H2NCH2CH2NH2 in MeOH, stirred with 5N NaOH, and treated with Br in CHCl3 at 0-8.degree. to give 2-(2-chloro-4-isopropylphenylimino)imidazolidine.HBr. The latter at 1 mg/kg in mice increased survival in a hypoxia screen from 40% (controls) to 70%.

IT **118955-15-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as CNS agent and cardio- and cytoprotectant)

RN 118955-15-0 CAPLUS
CN 1H-Imidazol-2-amine, N-[2-bromo-6-chloro-4-(1-methylethyl)phenyl]-4,5-dihydro-, monohydrobromide (9CI) (CA INDEX NAME)

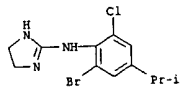
L3 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2002 ACS (Continued)



● HBr

IT **118854-98-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as CNS agent, cyto- and cardioprotectant)

RN 118854-98-1 CAPLUS
CN 1H-Imidazol-2-amine, N-[2-bromo-6-chloro-4-(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



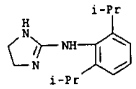
L3 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1985:593431 CAPLUS
DOCUMENT NUMBER: 103:193431
TITLE: Phenyliminoimidazolidines. Characterization of a class of potent agonists of octopamine-sensitive adenylate cyclase and their use in understanding the pharmacology of octopamine receptors
AUTHOR(S): Nathanson, James A.
CORPORATE SOURCE: Dep. Neurol., Harvard Med. Sch., Boston, MA, 02114, USA
SOURCE: Mol. Pharmacol. (1985), 28(3), 254-68
CODEN: MOPMA3; ISSN: 0026-895X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Approx. 30 substituted phenyliminoimidazolidines (PII) were examd. for agonist and antagonist effects on the highly enriched and specific octopamine (O)-sensitive adenylate cyclase (AC) present in the firefly light organ, as well as on ACs present in other invertebrate and vertebrate tissues. Several derivs. were extremely active and some had potencies exceeding those of any previously described agonists of O-sensitive AC. Stimulation by the potent PIIs was reversible, nonadditive to that caused by O, and could be antagonized by antagonists such as cyproheptadine, phentolamine, and propranolol. The inhibitory consts. agreed well with those for inhibiting O stimulation. Certain PII derivs. acted as partial agonists and some as antagonists of O stimulation. Structure-activity relationships revealed, among other things, that short-chain alkyl substitution in the 2- and 6-Phe positions enhanced activity, as did further substitution of 4-halo, 4-Me, or 4-hydroxy substituents. 4-Amino or N-alkyl substitution decreased activity. Structurally related benzylimidazoline derivs. such as tolazoline and naphazoline were partial O agonists, generally less active than the PIIs. Comparison, in 3 invertebrate species, of the effects of the PIIs and 2 other chem. classes of O agonists demonstrated clearcut differences in species responsiveness. Other comparative studies revealed that the agonist activity of the potent PIIs was specific for tissues contg. an O-sensitive AC; ACs activated by dopamine or by .beta.1- or .beta.2-adrenergic agonists were unaffected by these compds. The active PIIs affected a class of O receptors distinct from mammalian .alpha.1- or .alpha.2-adrenergic receptors. These O receptors also appeared distinct from mammalian 5-HT1 and 5-HT2 receptors. Correlative physiol. studies in insects revealed that the active PIIs mimicked O and were potent activators of light emission in the firefly light organ. The PIIs also cause disruption of motor and feeding behavior in tobacco hornworms, leading to insect death, an effect which was markedly potentiated by phosphodiesterase inhibitors.

IT **63346-74-7**
RL: BIOL (Biological study)
(octopamine-sensitive adenylate cyclase activation by, in light organ of firefly, structure in relation to)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

L3 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2002 ACS (Continued)



L3 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:447931 CAPLUS
DOCUMENT NUMBER: 87:47931
TITLE: Structure-activity relations and problems related to the mechanism of action of clonidine
AUTHOR(S): Rouot, Bruno; Leclerc, Gerard; Wermuth, Camille-Georges; Miesch, Francois; Schwartz, Jean
CORPORATE SOURCE: Fac. Pharm., Univ. Louis-Pasteur, Strasbourg, Fr.
SOURCE: J. Pharmacol. (1977), 8(1), 95-106
CODEN: JNPHAG
DOCUMENT TYPE: Journal
LANGUAGE: French
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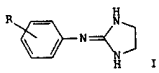
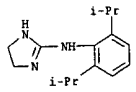


I

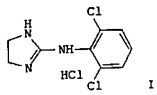
AB All 26 clonidine analogs (I) studied showed peripheral .alpha.-sympathomimetic activity, with IPS 56 (I; R = 2,3-dichloro) [15327-44-3] having the greatest hypertensive effect in demedullated rats. The results correlated with Es (steric const.) and F (sum of the field effect of the substituents) of the Hansch equation (1971). No such correlation was obsd. for hypotensive activity in intact rats. Compds. which had hypotensive activity also had high .alpha.-sympathomimetic activity, local anesthetic activity (rabbit cornea), and similar lipophilicity. However, the results were not sufficient to conclude that .alpha.-adrenergic mechanisms are involved in the hypotensive effects of clonidine and its analogs.

IT **63346-74-7**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(hypotensive and .alpha.-sympathomimetic activity of)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



L3 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1976:456532 CAPLUS
DOCUMENT NUMBER: 85:56532
TITLE: Clonidine and related analogues. Quantitative correlations
AUTHOR(S): Rouot, Bruno; Leclerc, Gerard; Wermuth, Camille G.; Miesch, Francois; Schwartz, Jean
CORPORATE SOURCE: Fac. Pharm., Univ. Louis Pasteur, Strasbourg, Fr.
SOURCE: J. Med. Chem. (1976), 19(8), 1049-54
CODEN: JMCMAR
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

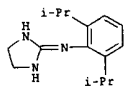


I

AB A series of 22 derivs. of clonidine-HCl (I) [4205-91-8] were prepd. by the cyclization reaction of ethylenediamine with an S-methylisothiouronium salt deriv. and the main physicochem. parameters (log P, .DELTA.RM, pKa) detd. Quant. correlations between peripheral .alpha.-mimetic action (pithed rats) and physicochem. parameters pointed out the crit. role of the steric effect of ortho substituents. Attempted quant. correlations between physicochem. parameters and central hypotensive activity were unsuccessful. The mechanism of action of I is discussed.

IT **59465-43-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and blood pressure response to)

RN 59465-43-9 CAPLUS
CN Benzenamine, N-2-imidazolidinylidene-2,6-bis(1-methylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L3 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2002 ACS (Continued)

=> log y

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NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 09	JAPIO to be reloaded August 25, 2002
NEWS 20	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 21	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 22	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded

NEWS EXPRESS	February 1 CURRENT WINDOWS VERSION IS V6.0d, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
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NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
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http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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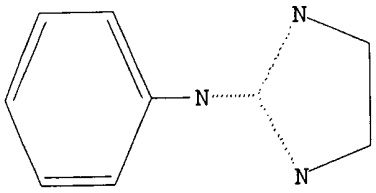

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100.0% PROCESSED 990 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

Examiner Anderson 703-605-1157

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 17913 TO 21687
PROJECTED ANSWERS: 4943 TO 7017

L2 50 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 12:12:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20061 TO ITERATE

100.0% PROCESSED 20061 ITERATIONS 5848 ANSWERS
SEARCH TIME: 00.00.02

L3 5848 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	140.28	140.49

FILE 'CAPLUS' ENTERED AT 12:12:46 ON 21 AUG 2002
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 21 Aug 2002 VOL 137 ISS 8
FILE LAST UPDATED: 20 Aug 2002 (20020820/ED)

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=> s l3
L4 9033 L3

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.40	140.89

FILE 'REGISTRY' ENTERED AT 12:12:55 ON 21 AUG 2002
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STRUCTURE FILE UPDATES: 20 AUG 2002 HIGHEST RN 444542-98-7
DICTIONARY FILE UPDATES: 20 AUG 2002 HIGHEST RN 444542-98-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

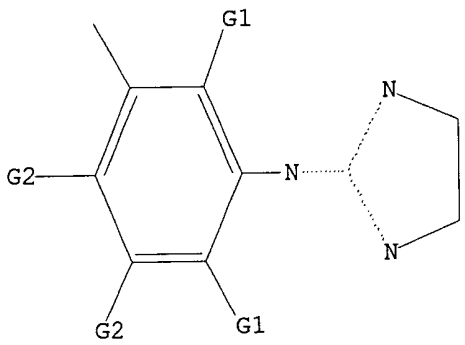
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10058456.str

L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR



G1 H,X,O,C
G2 C,H,X

Structure attributes must be viewed using STN Express query preparation.

=> s l5 subset=l3 full
FULL SUBSET SEARCH INITIATED 12:15:46 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 5848 TO ITERATE

100.0% PROCESSED 5848 ITERATIONS 3794 ANSWERS
SEARCH TIME: 00.00.01

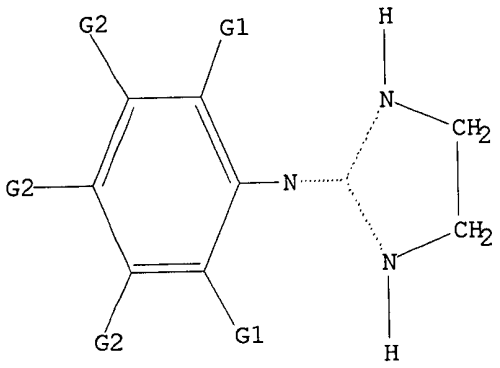
L6 3794 SEA SUB=L3 SSS FUL L5

=>
Uploading 10058456.str

Examiner Anderson 703-605-1157

L7 STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7 STR



G1 H,X,O,C

G2 C,H,X

Structure attributes must be viewed using STN Express query preparation.

=> s l7 subset=l5 full
L5 MAY NOT BE USED HERE
The L-number must have been created by a search in this file. To see all L-numbers defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>). For additional information on subset searching in this file, enter HELP SUBSET.
ENTER SUBSET L# OR (END):6
6 IS NOT A VALID L#
L-numbers must be in the range L1-L999.
ENTER SUBSET L# OR (END):16
FULL SUBSET SEARCH INITIATED 12:17:26 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 3794 TO ITERATE

100.0% PROCESSED 3794 ITERATIONS 1495 ANSWERS
SEARCH TIME: 00.00.01

L8 1495 SEA SUB=L6 SSS FUL L7

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	69.14	210.03

FILE 'CAPLUS' ENTERED AT 12:17:37 ON 21 AUG 2002
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FILE COVERS 1907 - 21 Aug 2002 VOL 137 ISS 8
FILE LAST UPDATED: 20 Aug 2002 (20020820/ED)

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=> s l8
L9 7548 L8

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.19	211.22

FILE 'REGISTRY' ENTERED AT 12:19:37 ON 21 AUG 2002
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DICTIONARY FILE UPDATES: 20 AUG 2002 HIGHEST RN 444542-98-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

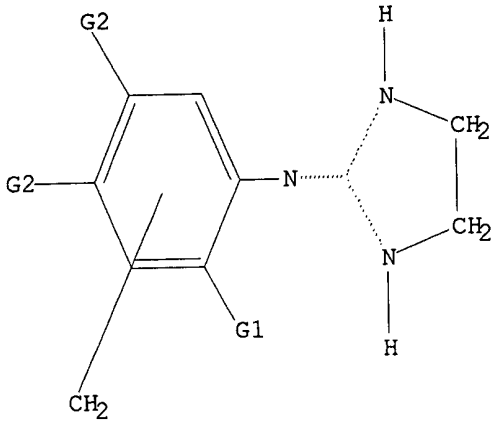
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10058456.str

L10 STRUCTURE UPLOADED

=> d
L10 HAS NO ANSWERS
L10 STR



G1 H,X,O,C

G2 C,H,X

Structure attributes must be viewed using STN Express query preparation.

=> s l10 subset=l8 full
FULL SUBSET SEARCH INITIATED 12:20:03 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1495 TO ITERATE

100.0% PROCESSED 1495 ITERATIONS 218 ANSWERS
SEARCH TIME: 00.00.01

L11 218 SEA SUB=L8 SSS FUL L10

=> fil caplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	33.43	244.65

FILE 'CAPLUS' ENTERED AT 12:20:07 ON 21 AUG 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 21 Aug 2002 VOL 137 ISS 8
FILE LAST UPDATED: 20 Aug 2002 (20020820/ED)

This file contains CAS Registry Numbers for easy and accurate

substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

```
=> s l11
L12         328 L11

=> s l12 and urinary
         107190 URINARY
L13           2 L12 AND URINARY

=> d ibib abs hitstr 1-2
```

L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS

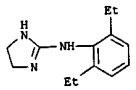
ACCESSION NUMBER: 1997:318325 CAPLUS
DOCUMENT NUMBER: 127:13229
TITLE: The peripheral action of clonidine analog ST-91: involvement of atrial natriuretic factor
AUTHOR(S): Gutkowska, Jolanta; Mukaddam-Daher, Suhayla; Tremblay, Johanne
CORPORATE SOURCE: Laboratory Cardiovascular Biochemistry, Centre Recherche Hotel-Dieu Montreal, Universite Montreal, Montreal, QC, H2W 1T8, Can.
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1997), 281(2), 670-676
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB It is generally thought that the cardiovascular and renal effects of clonidine, an alpha-2 adrenergic agonist, are mediated by central mechanisms. Our previous work has shown that diuresis and natriuresis caused by central administration of clonidine are mediated by an enhanced release of atrial natriuretic factor (ANF). Because clonidine has been shown to have peripheral actions the objective of the present study was to det. whether ANF is also involved in these actions. Studies were performed with use of a structural clonidine analog. ST-91, which does not cross the blood-brain barrier. I.v. injection of various doses (0-250 .mu.g/rat) of ST-91 into conscious, normally hydrated female Sprague-Dawley rats (200-250 g) produced dose-related increases in **urinary** output, which were accompanied by significant increases in **urinary** sodium, potassium and cGMP excretion. Compared with saline, the highest dose of ST-91 (250 .mu.g/rat) during the first hour of treatment significantly (P < .001, n = 18) enhanced **urinary** output (0.2 .+-. 0.1 vs. 3.0 .+-. 1.1 mL/h) and excretion of sodium (28 .+-. 4 vs. 345 .+-. 50 .mu.mol/h), potassium (10 .+-. 4 vs. 165 .+-. 37 .mu.mol/h) and cGMP (191 .+-. 29 vs. 1340 .+-. 322 pmol/h), the biol. marker of ANF. These renal responses were assocd. with increased plasma ANF (59 .+-. 28 pg/mL, P < .001, n = 12), measured 10 min after ST-91 (250 .mu.g/rat), which remained elevated for at least 1 h (P < .01, n = 6). The enhanced renal responses that were induced by 10 .mu.g ST-91 were partially, yet significantly inhibited by yohimbine (50 .mu.g), an alpha-2 antagonist. On the other hand, efaroxan (500 .mu.g), an I1 imidazoline receptor antagonist, showed a stronger inhibitory effect, whereas naloxone (0.8 mg) had no effect. Pretreatment of rats with anti-ANF reduced the diuretic and natriuretic effects of ST-91. These results indicate that the renal effects of ST-91 are mediated by imidazoline as well as by alpha-2 adrenergic receptors, but not by opioid receptors. Furthermore, the renal effects evoked by ST-91 are mediated by ANF.

IT **4749-61-5**, ST-91
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(peripheral action of clonidine analog ST-91: involvement of atrial natriuretic factor)

RN 4749-61-5 CAPLUS
CN 1H-Imidazol-2-amine, N-(2,6-diethylphenyl)-4,5-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



● HCl

L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS

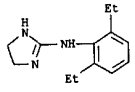
ACCESSION NUMBER: 1990:1110 CAPLUS
DOCUMENT NUMBER: 112:1110
TITLE: .alpha.2-Adrenergic receptors and the sodium/hydrogen ion exchanger in the intestinal epithelial cell line, HT-29
AUTHOR(S): Cantiello, Horacio F.; Lanier, Stephen M.
CORPORATE SOURCE: Massachusetts Gen. Hosp., Harvard Med. Sch., Boston, MA, 02114, USA
SOURCE: J. Biol. Chem. (1989), 264(27), 16000-7
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effect of .alpha.2-adrenergic receptors (.alpha.2-AR) activation on basal and stimulated Na+/H+ exchange was studied in epithelial cells isolated from human colon (HT-29 adenocarcinoma cells). Na+/H+ exchange was measured by quantitation of intracellular H+ ion concn. (acetoxymethyl ester 2,7-biscarboxyethyl-5(6)carboxyfluorescein) and 22Na+ uptake. HT-29 cells expressed an amiloride-sensitive Na+/H+ exchanger that was activated by redn. of intracellular pH (pHi) to 6.0 but was quiescent at a physiol. pHi. The rapid alkalination obsd. after acid loading (0.57 pH units/min/10⁴ cells) was dependent on external Na and was blocked by amiloride (Ki .apprx.2.1 .mu.M). Although epinephrine and the selective .alpha.2-AR agonists clonidine and UK-14304 inhibited forskolin-activated adenylyl cyclase, these compds. did not alter basal Na+/H+ exchange. Stimulated Na+/H+ exchange was similarly unaffected by epinephrine. In contrast, stimulated Na+/H+ exchanger activity was completely inhibited by the selective .alpha.2-agonists clonidine, UK-14304, and guanabenz. This inhibitory effect was not blocked by the .alpha.2-AR antagonist rauwolscine, and it is likely due to a direct interaction with the exchanger mol. itself. Structure/activity studies indicated that the compds. inhibiting exchanger activity possess either an imidazoline or guanidinium moiety. Although these mols. bear structural similarity to amiloride, they did not inhibit the amiloride-sensitive epithelial Na channel in toad **urinary** bladder, suggesting that these compds. may be useful as amiloride-like ligands selective for the Na+/H+ exchanger. Evidently, in the HT-29 intestinal cell line, in contrast to observations in other tissues, .alpha.2-AR are not coupled to the Na+/H+ exchanger, suggesting that the cell-signaling mechanisms utilized by the .alpha.2-AR are tissue specific.

IT **4749-61-5**, ST-91
RL: BIOL (Biological study)
(hydrogen ion-sodium exchange transport inhibition by, in intestine epithelial cells of human, structure in relation to)

RN 4749-61-5 CAPLUS
CN 1H-Imidazol-2-amine, N-(2,6-diethylphenyl)-4,5-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS (Continued)



● HCl

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.59	256.24
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.24	-1.24

FILE 'STNGUIDE' ENTERED AT 12:21:56 ON 21 AUG 2002
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Aug 16, 2002 (20020816/UP).

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.06	256.30
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.24

FILE 'REGISTRY' ENTERED AT 12:22:21 ON 21 AUG 2002
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STRUCTURE FILE UPDATES: 20 AUG 2002 HIGHEST RN 444542-98-7
DICTIONARY FILE UPDATES: 20 AUG 2002 HIGHEST RN 444542-98-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

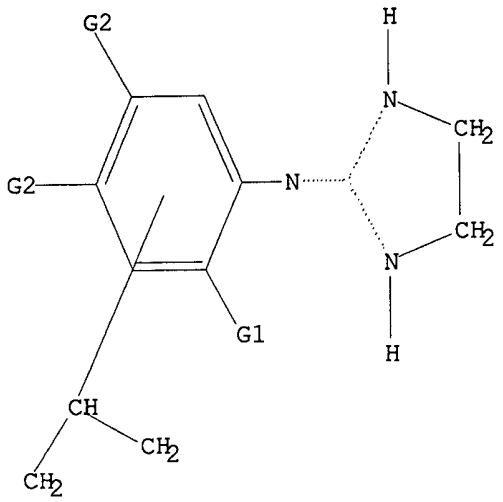
Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 10058456.str

L14 STRUCTURE UPLOADED

=> d
L14 HAS NO ANSWERS
L14 STR



G1 H,X,O,C

G2 C,H,X

Structure attributes must be viewed using STN Express query preparation.

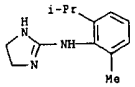
=> s l14 subset=l8 full
FULL SUBSET SEARCH INITIATED 12:23:38 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1495 TO ITERATE

100.0% PROCESSED 1495 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L15 4 SEA SUB=L8 SSS FUL L14

=> d scan

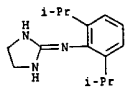
L15 4 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazol-2-amine, 4,5-dihydro-N-[2-methyl-6-(1-methylethyl)phenyl]-(9CI)
MF C13 H19 N3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

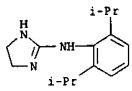
L15 4 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzenamine, N-2-imidazolidinylidene-2,6-bis(1-methylethyl)-, monohydrochloride (9CI)
MF C15 H23 N3 . Cl H



● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

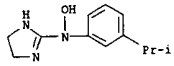
L15 4 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI)
MF C15 H23 N3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L15 4 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Imidazol-2-amine, 4,5-dihydro-N-hydroxy-N-[3-(1-methylethyl)phenyl]-, monohydrochloride (9CI)
MF C12 H17 N3 O . Cl H



● HCl

ALL ANSWERS HAVE BEEN SCANNED

```
=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                    34.19      290.49

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY     SESSION
CA SUBSCRIBER PRICE                                     0.00       -1.24

FILE 'CAPLUS' ENTERED AT 12:23:57 ON 21 AUG 2002
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FILE COVERS 1907 - 21 Aug 2002  VOL 137 ISS 8
FILE LAST UPDATED: 20 Aug 2002  (20020820/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

CAS roles have been modified effective December 16, 2001. Please
check your SDI profiles to see if they need to be revised. For
information on CAS roles, enter HELP ROLES at an arrow prompt or use
the CAS Roles thesaurus (/RL field) in this file.

=> s l15
L16         10 L15

=> d ibib abs hitstr 1-10
```
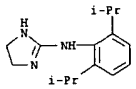

L16 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:883550 CAPLUS
DOCUMENT NUMBER: 136:320707
TITLE: Three-Dimensional common-Feature hypotheses for octopamine agonist 2-(arylimino)imidazolidines
AUTHOR(S): Hirashima, Akinori; Morimoto, Masako; Kuwano, Eiichi; Taniguchi, Eiji; Eto, Morifusa
CORPORATE SOURCE: Department of Applied Genetics and Pest Management, Kyushu University, Faculty of Agriculture, Graduate School, Fukuoka, Higashi-ku, 812-8581, Japan
SOURCE: Bioorganic & Medicinal Chemistry (2001), Volume Date 2002, 10(1), 117-123
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Three-dimensional pharmacophore hypotheses were built from a set of 10 octopamine (OA) agonist 2-(Arylimino)imidazolidines (AIIs), 2-(Arylimino)thiazolidines (AITs) and 2-(Arylimino)oxazolidines (AIOs). OA agonist activities were detd. using the adenylate cyclase assay in American cockroaches (P. americana). Among the 10 common-featured models generated by program Catalyst/HipHop, a hypothesis including a ring arom. (RA), a pos. ionizable (PI) and three hydrophobic aliph. (HpAl) features was considered to be important in evaluating the OA-agonist activity. Active OA agonist 2,6-Et2 AII mapped well onto all the RA, PI and HpAl features of the hypothesis. On the other hand, less active compds. were shown to be difficult to achieve the energetically favorable conformation which is found in the active mols. in order to fit the 3-D common-feature pharmacophore models. Taken together, 2,6-Et2-Ph and foramidine structures are important as OA agonists. The present studies on OA agonists demonstrate that a RA, a PI and three HpAl sites located on the mol. seem to be essential for OA-agonist activity.

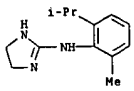
IT **63346-74-7 359668-33-0**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(QSAR for octopamine agonist (arylimino)imidazolidines)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 359668-33-0 CAPLUS
CN 1H-Imidazol-2-amine, 4,5-dihydro-N-[2-methyl-6-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

L16 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2002 ACS (Continued)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

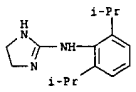
L16 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:596828 CAPLUS
DOCUMENT NUMBER: 135:222824
TITLE: Identification of novel inhibitors of calling and in vitro [14C]acetate incorporation by pheromone glands of Plodia interpunctella
AUTHOR(S): Hirashima, Akinori; Eiraku, Tomohiko; Watanabe, Yasuyuki; Kuwano, Eiichi; Taniguchi, Eiji; Eto, Morifusa
CORPORATE SOURCE: Department of Applied Genetics and Pest Management, Faculty of Agriculture, Graduate School, Kyushu University, Fukuoka, 812-8581, Japan
SOURCE: Pest Management Science (2001), 57(8), 713-720
CODEN: PMSCFC; ISSN: 1526-498X
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

SB599.P47 (e-journal)

AB Some octopamine agonists were found to suppress in vitro biosynthesis of the calling pheromone of the Indian meal moth, Plodia interpunctella. Isolated pheromone-gland prepns. incorporated sodium [14C]acetate at a linear rate for 3h when incubated with the pheromone biosynthesis activating neuropeptide (PBAN). This incorporation was dependent on the dose of PBAN (up to 0.5 .mu.M). Thin-layer chromatog. of a pheromone-gland ext. revealed quant. incorporation of radioactivity into a product exhibiting the same mobility as (Z,E)-9,12-tetradecadienyl acetate, the main component of the calling pheromone of P. interpunctella. Twenty-seven octopamine agonists were initially screened using a calling behavior bioassay of female P interpunctella. Four derivs. with activity in the nanomolar range were identified which were, in order of decreasing pheromonostatic activity: 2-(2,6-diethylphenylimino)thiazolidine > 2-(2,6-diethylphenylimino)oxazolidine > 2-(2,6-dimethylphenylimino)thiazolidine > 2-(2-ethylphenylimino)oxazolidine. These compds. also showed in vitro inhibitory activity in intracellular de novo pheromone biosynthesis. The results of the present study indicate that these derivs. could provide useful information in the characterization and differentiation of octopaminergic receptor types and subtypes.

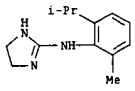
IT **63346-74-7P 359668-33-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and pheromonostatic activity of)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 359668-33-0 CAPLUS
CN 1H-Imidazol-2-amine, 4,5-dihydro-N-[2-methyl-6-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

L16 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2002 ACS (Continued)



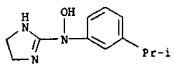
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:37784 CAPLUS
DOCUMENT NUMBER: 134:231513
TITLE: Synthesis, structure, and binding of some 2-imidazolines to rat brain alfa-1 and alfa-2-adrenergic receptors
AUTHOR(S): Saczewski, F.; Kobierska, E.; Debowski, T.; Charakchiewa-Minol, S.; Mokrosz, M.; Gdaniec, M.; Nowak, E.
CORPORATE SOURCE: Department of Chemical Technology of Drug and Organic Chemistry, Medical University of Gdansk, Pol.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (2000), 333(12), 425-430
CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:231513

AB A series of novel 2-[(2-aminophenyl)imino]imidazolinium salts and N-benzyl-N-(4,5-dihydro-imidazol-2-yl)-O-methylhydroxylamine hydrochloride were prepd. and their structure was detd. by IR and NMR spectroscopic data as well as X-ray anal. of the imidazolinium azide salt of one of the compds. Binding evaluation for both .alpha.1- and .alpha.2-adrenergic receptors in rat brain prepns. of these compds. and previously described .alpha.-hydroxy-2-aryliminoimidazolines 11a-d, N-(4,5-dihydroimidazol-2-yl)-1,3-2-oxodihydrobenzimidazoles, 2-amino-N-(4,5-dihydroimidazol-2-yl)-benzimidazoles, and N-(4,5-dihydroimidazol-2-yl)-indoles was performed. Among the compds. tested, 2-[(2-amino-4,5-dichlorophenyl)imino]imidazolini um chloride showed highest binding affinity to .alpha.2-adrenoreceptors (Ki = 30 nM).

IT **330685-57-9**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(synthesis, structure, and binding of imidazolines to brain .alpha.1- and .alpha.2-adrenergic receptors)

RN 330685-57-9 CAPLUS
CN 1H-Imidazol-2-amine, 4,5-dihydro-N-hydroxy-N-[3-(1-methylethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

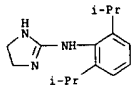
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:142505 CAPLUS
DOCUMENT NUMBER: 132:330832
TITLE: Three-dimensional molecular field analyses of octopaminergic agonists and antagonists for the locust neuronal octopamine receptor class 3
AUTHOR(S): Hirashima, A.; Nagata, T.; Pan, C.; Kuwano, E.; Taniguchi, E.; Eto, M.
CORPORATE SOURCE: Graduate School, Division of Bioresource and Bioenvironmental Sciences, Kyushu University, Fukuoka, Japan
SOURCE: Journal of Molecular Graphics & Modelling (2000), Volume Date 1999, 17(3/4), 198-206
CODEN: JMGMFI; ISSN: 1093-3263
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The quant. structure-activity relationship (QSAR) of a set of 70 octopaminergic agonists and 20 antagonists against octopamine receptor class 3 (OAR3) in locust nervous tissue was analyzed by mol. field anal. (MFA). MFA of these compds. evaluated effectively the energy between a probe and a mol. model at a series of points defined by a rectangular grid. Contour surfaces for the mol. fields are presented. These results provide useful information in the characterization and differentiation of octopaminergic receptor types and subtypes.

IT **63346-74-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(three-dimensional mol. field analyses of octopaminergic agonists and antagonists for locust neuronal octopamine receptor class 3)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



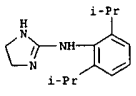
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:138409 CAPLUS
DOCUMENT NUMBER: 132:260196
TITLE: Prediction of distribution coefficients from structure. Comparison of calculated and experimental data for various drugs
AUTHOR(S): Tsantili-Kakoulidou, A.; Panderi, I.; Piperaki, S.; Csizmadia, F.; Darvas, F.
CORPORATE SOURCE: Department of Pharmacy, University of Athens, Athens, 157 71, Greece
SOURCE: European Journal of Drug Metabolism and Pharmacokinetics (1999), 24(3), 205-212
CODEN: EJDPD2; ISSN: 0378-7966
PUBLISHER: Medecine et Hygiene
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The efficiency of the program PrologD to predict distribution coeffs. (D) at any pH and pairing ion concn. has been tested using exptl. logD values for various drugs measured under std. conditions of buffers and ionic strength. Clonidine derivs., fluoroquinolones and .beta.-blockers were included as particular pharmacol. classes within the testing data set. Calcns. were performed using the three logP estn. options implemented in the program. PrologD proved to be very efficient and can be of great advantage in drug research. Prediction patterns and correlations between exptl. and calcd. data indicate acceptable results for more than 80% of the data. In addn., comparable studies using the different options permitted suggestions for the more suitable logP estn. method in respect of the particular classes of compds.

IT **63346-74-7**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(comparison of calcd. and exptl. data for various drugs in prediction of distribution coeffs. from structure)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



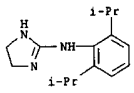
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:669819 CAPLUS
DOCUMENT NUMBER: 127:274156
TITLE: Neurotransmitter-receptors as targets for new insecticides
AUTHOR(S): Roeder, T.; Degen, J.; Dyczkowski, C.; Gewecke, M.
CORPORATE SOURCE: Zoologisches Insitut, Universitat Hamburg, Neurophysiologie, Hamburg, D-20146, Germany
SOURCE: New Strategies in Locust Control (1997), 219-223.
Editor(s): Krall, S.; Peveling, R.; Ba Diallo, D.
Birkhaeuser: Basel, Switz.
CODEN: 65EDA4
DOCUMENT TYPE: Conference
LANGUAGE: English

AB The locust neuronal octopamine receptor is believed to be an ideal target for highly specific insecticides. The authors characterized a no. of high affinity agonists of this receptor subtype. Using structure-activity relationships, the authors were able to optimize the structure of these compds. in terms of their affinities. A variety of these compds. show a high degree of specificity for insect octopamine receptors vs. vertebrate adrenergic receptors. The high affinity together with the high degree of specificity makes compds. such as the phenyliminoimidazolidines ideal starting points for the development of new insecticides.

IT **63346-74-7**, NC 20
RL: BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
(affinity for locust neuronal octopamine receptor)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

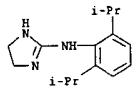


L16 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:303934 CAPLUS
DOCUMENT NUMBER: 122:77274
TITLE: Pharmacology of the octopamine receptor from locust central nervous tissue (OAR3)
AUTHOR(S): Roeder, Thomas
CORPORATE SOURCE: Zool. Inst., Univ. Hamburg, Hamburg, D-20146, Germany
SOURCE: British Journal of Pharmacology (1995), 114(1), 210-16
CODEN: BJPCBM; ISSN: 0007-1188
PUBLISHER: Stockton
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The present study characterized highly effective agonists from different classes of compds. for the neuronal octopamine receptor (OAR3) of the migratory locust (Locusca migratoria L.). Biogenic amines and phenyliminoimidazolidines (PIIs) were employed for the study of structure-activity relationships. The highest affinity PIIs were predominantly those with the substitutions at the positions 2 and 4 of the phenolic ring (e.g. NC 7, K1 = 0.3 nM, NC8, KI = 0.81 nM). Substitutions at these positions always had pos. effectives on the affinity of the resp. agonists. Substitutions at the positions 3, 5 and 6, however, always had neg. effects on the affinity. At the position one of the phenolic ring, heterocyclic substituents are preferred. Some PIIs had a more than 30 times higher affinity for OARs than for .alpha.-adrenoceptors which are the vertebrate homologues of the insect octopamine receptors. The only non-PII with subnanomolar affinity was the aminooxazlline deriv. AC 6 (K1 = 0.92 nM). A variety of substances with known insecticidal activity such as chlordimeform, demethylchlordimeform, amitraz or AC 6 had high affinity for the locust neuronal octopamine receptor.

IT **63346-74-7**, NC 20
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(structure-activity relationship of agonists for locust neuronal octopamine receptor)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



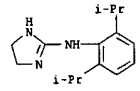
L16 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1985:593431 CAPLUS
DOCUMENT NUMBER: 103:193431
TITLE: Phenyliminoimidazolidines. Characterization of a class of potent agonists of octopamine-sensitive adenylate cyclase and their use in understanding the pharmacology of octopamine receptors
AUTHOR(S): Nathanson, James A.
CORPORATE SOURCE: Dep. Neurol., Harvard Med. Sch., Boston, MA, 02114, USA
SOURCE: Mol. Pharmacol. (1985), 28(3), 254-68
CODEN: MOPMA3; ISSN: 0026-895X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Approx. 30 substituted phenyliminoimidazolidines (PII) were examd. for agonist and antagonist effects on the highly enriched and specific octopamine (O)-sensitive adenylate cyclase (AC) present in the firefly light organ, as well as on ACs present in other invertebrate and vertebrate tissues. Several derivs. were extremely active and some had potencies exceeding those of any previously described agonists of O-sensitive AC. Stimulation by the potent PIIs was reversible, nonadditive to that caused by O, and could be antagonized by antagonists such as cyproheptadine, phentolamine, and propranolol. The inhibitory consts. agreed well with those for inhibiting O stimulation. Certain PII derivs. acted as partial agonists and some as antagonists of O stimulation. Structure-activity relationships revealed, among other things, that short-chain alkyl substitution in the 2- and 6-Phe positions enhanced activity, as did further substitution of 4-halo, 4-Me, or 4-hydroxy substituents. 4-Amino or N-alkyl substitution decreased activity. Structurally related benzylimidazoline derivs. such as tolazoline and naphazoline were partial O agonists, generally less active than the PIIs. Comparison, in 3 invertebrate species, of the effects of the PIIs and 2 other chem. classes of O agonists demonstrated clearcut differences in species responsiveness. Other comparative studies revealed that the agonist activity of the potent PIIs was specific for tissues contg. an O-sensitive AC; ACs activated by dopamine or by .beta.1- or .beta.2-adrenergic agonists were unaffected by these compds. The active PIIs affected a class of O receptors distinct from mammalian .alpha.1- or .alpha.2-adrenergic receptors. These O receptors also appeared distinct from mammalian 5-HT1 and 5-HT2 receptors. Correlative physiol. studies in insects revealed that the active PIIs mimicked O and were potent activators of light emission in the firefly light organ. The PIIs also cause disruption of motor and feeding behavior in tobacco hornworms, leading to insect death, an effect which was markedly potentiated by phosphodiesterase inhibitors.

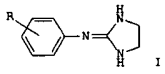
IT **63346-74-7**
RL: BIOL (Biological study)
(octopamine-sensitive adenylate cyclase activation by, in light organ of firefly, structure in relation to)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)

L16 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2002 ACS (Continued)



L16 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:447931 CAPLUS
DOCUMENT NUMBER: 87:47931
TITLE: Structure-activity relations and problems related to the mechanism of action of clonidine
AUTHOR(S): Rouot, Bruno; Leclerc, Gerard; Wermuth, Camille-Georges; Miesch, Francois; Schwartz, Jean
CORPORATE SOURCE: Fac. Pharm., Univ. Louis-Pasteur, Strasbourg, Fr.
SOURCE: J. Pharmacol. (1977), 8(1), 95-106
CODEN: JNPHAG
DOCUMENT TYPE: Journal
LANGUAGE: French
GI

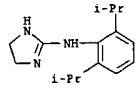


I

AB All 26 clonidine analogs (I) studied showed peripheral .alpha.-sympathomimetic activity, with IPS 56 (I; R = 2,3-dichloro) [15327-44-3] having the greatest hypertensive effect in demedullated rats. The results correlated with Es (steric const.) and F (sum of the field effect of the substituents) of the Hansch equation (1971). No such correlation was obsd. for hypotensive activity in intact rats. Compds. which had hypotensive activity also had high .alpha.-sympathomimetic activity, local anesthetic activity (rabbit cornea), and similar lipophilicity. However, the results were not sufficient to conclude that .alpha.-adrenergic mechanisms are involved in the hypotensive effects of clonidine and its analogs.

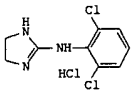
IT **63346-74-7**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(hypotensive and .alpha.-sympathomimetic activity of)

RN 63346-74-7 CAPLUS
CN 1H-Imidazol-2-amine, N-[2,6-bis(1-methylethyl)phenyl]-4,5-dihydro- (9CI) (CA INDEX NAME)



L16 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:456532 CAPLUS
DOCUMENT NUMBER: 85:56532
TITLE: Clonidine and related analogues. Quantitative correlations
AUTHOR(S): Rouot, Bruno; Leclerc, Gerard; Wermuth, Camille G.; Miesch, Francois; Schwartz, Jean
CORPORATE SOURCE: Fac. Pharm., Univ. Louis Pasteur, Strasbourg, Fr.
SOURCE: J. Med. Chem. (1976), 19(8), 1049-54
CODEN: JMCMAR
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

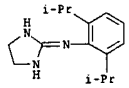


I

AB A series of 22 derivs. of clonidine-HCl (I) [4205-91-8] were prepd. by the cyclization reaction of ethylenediamine with an S-methylisothiouronium salt deriv. and the main physicochem. parameters (log P, .DELTA.RM, pKa) detd. Quant. correlations between peripheral .alpha.-mimetic action (pithed rats) and physicochem. parameters pointed out the crit. role of the steric effect of ortho substituents. Attempted quant. correlations between physicochem. parameters and central hypotensive activity were unsuccessful. The mechanism of action of I is discussed.

IT **59465-43-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and blood pressure response to)

RN 59465-43-9 CAPLUS
CN Benzenamine, N-2-imidazolidinylidene-2,6-bis(1-methylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L16 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2002 ACS (Continued)

=> FIL STNGUIDE

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	49.43	339.92

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.20	-7.44

FILE 'STNGUIDE' ENTERED AT 12:32:21 ON 21 AUG 2002

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Aug 16, 2002 (20020816/UP).

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.06	339.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-7.44

STN INTERNATIONAL LOGOFF AT 12:32:51 ON 21 AUG 2002